

3.2 Rationale

It is difficult to visualise patterns in the responses of whole sets of variables simultaneously. Each variable can be considered a dimension, with its own story to tell in terms of its mean, variance, skewness, etc. For most sets of multivariate data, there are also correlations among the variables. *Ordination* is simply the ordering of samples in Euclidean space (e.g., on a page) in some way, using the information provided by the variables. The primary goal of ordination methods is usually to reduce the dimensionality of the data cloud in order to allow the most salient patterns and structures to be observed.

Different ordination methods have different criteria by which the picture in reduced space is drawn (see chapter 9 of [Legendre & Legendre \(1998\)](#) for a more complete discussion). For example:

- Non-metric multi-dimensional scaling (MDS) preserves the rank order of the inter-point dissimilarities (for whatever resemblance measure has been chosen) as well as possible within the constraints of a small number of dimensions (usually just two or three). The adequacy of the plot is ascertained by virtue of how well the inter-point distances in the reduced-dimension, Euclidean ordination plot reflect the rank orders of the underlying dissimilarities (see, for example, chapter 5 in [Clarke & Warwick \(2001\)](#)).
- Principal components analysis (PCA) is a *projection* of the points (perpendicularly) onto axes that minimise residual variation in *Euclidean space*. The first principal component axis is defined as the straight line drawn through the cloud of points such that the variance of sample points, when projected perpendicularly onto the axis, is *maximised* (see, for example, chapter 4 of [Clarke & Warwick \(2001\)](#)).
- Correspondence analysis (CA) is also a projection of the points onto axes that minimise residual variation, but this is done in the space defined by the *chi-squared distances* among points ([ter Braak \(1987\)](#) , [Minchin \(1987\)](#) , [Legendre & Legendre \(1998\)](#));
- Principal coordinates analysis (PCO) is like MDS in that it is very flexible – it can be based on any (symmetric) resemblance matrix. However, it is also like a PCA, in that it is a *projection* of the points onto axes that minimise residual variation *in the space of the resemblance measure chosen*.

PCO performed on a resemblance matrix of Euclidean distances reproduces the pattern and results that would be obtained by a PCA on the original variables. Similarly, PCO performed on a resemblance matrix of chi-squared distances reproduces the pattern that would be obtained by a CA on the original variables. Thus, PCO is a more general procedure than either PCA or CA, yielding a projection in the space indicated by the resemblance measure chosen.

Two other features of PCO serve to highlight its affinity with PCA (as a projection). First, the scales of the resulting PCO axes are interpretable in the units of the original resemblance measure. Although the distances between samples in a plot of few dimensions will underestimate the distances in the full-dimensional space, they are, nevertheless, estimated in the same units as the original resemblance measure, but as projected along the PCO axes. Thus, unlike MDS axes, the PCO axes refer to a non-arbitrary quantitative scale defined by the chosen resemblance measure.

Second, PCO axes (like PCA axes) are centered at zero and are only defined up to their sign. So, any PCO axis can be reflected (by changing the signs of the sample scores), if convenient⁶¹.

For many multivariate applications (especially for species abundance data), MDS is usually the most appropriate ordination method to use for visualising patterns in a small number of dimensions, because it is genuinely the most flexible and robust approach available ([Kenkel & Orloci \(1986\)](#) , [Minchin \(1987\)](#)). There is a clear relationship in the philosophy underlying the ANOSIM testing procedure and non-metric MDS in PRIMER. Both are non-parametric approaches that work on the ranks of resemblance measures alone. However, when using PERMANOVA to perform a partitioning for more complex designs, it is the actual dissimilarities (and not just their ranks) that are of interest and which are being modeled directly (e.g., see the section [PERMANOVA versus ANOSIM](#) in [chapter 1](#)). Therefore, we may wish to use an ordination procedure that is a little more consistent with this philosophy, and PCO may do this by providing a direct projection of the points in the space defined by the actual dissimilarities themselves. Although MDS will provide a more optimal solution for visualising in a few dimensions what is happening in the multi-dimensional cloud, the PCO can in some cases provide additional insights regarding original dissimilarities that might be lost in the non-metric MDS, due to ranking. In addition (as stated in [chapter 2](#)), the Euclidean distance between two points in the space defined by the full set of PCO axes (all together) is equivalent to the original dissimilarity between those two points using the chosen resemblance measure on the original variables⁶². So another main use of PCO axes is to obtain *distances among centroids*, which can then form the basis of further analyses when dealing with more complex and/or large multi-factorial datasets.

⁶¹ This is done within PRIMER in the same manner as for either an MDS or PCA plot, by choosing **Graph > Flip X** or **Graph > Flip Y** in the resulting configuration.

⁶² With appropriate separate treatment of the axes corresponding to the positive and negative eigenvalues, if any, see [McArdle & Anderson \(2001\)](#) and [Anderson \(2006\)](#) and the section on [Negative eigenvalues](#) for details.